2024

Second Quarter

PTC Newsletter

PTC Polymer Technology Consortia

UPCOMING EVENTS

Mark Your Calendars for the PTC Fall meetings!

Scratch Behavior of Polymers Consortium-SCRATCH

SCRATCH FALL meeting-October 17th, 2024 at Texas A&M University

Polymer Technology Industrial Consortium-PTIC

PTIC FALL meeting—October 17th-18th, 2024
Both meetings at Texas A&M University-College Station, TX

Inside the Newsletter

Pavan Kolluru

Simultaneously Tougher and Thermally More Stable Hydrogen Bonded Polymer Glasses

Dr. Pavan Kolluru is an Assistant Professor in the Materials Science and Engineering Department, and his research group aims to understand the mechanical behavior of polymers, particularly at the sub-micron length scales. One current area of focus in the group is to understand the role of the relatively weak dynamic non-covalent bonds such as H-bonds in improving orthogonal mechanical properties such as the strength (σ_f) and toughness (U_T) of glassy state polymers. In fact, only a handful of studies, all focusing on semicrystalline polyvinyl alcohol (PVA), have been able to show simultaneous improvements in strength and toughness [1-4]. However, as depicted in Figure 1, optimal values of σ_f and U_T (shown using shaded ovals) in these studies were observed to be accompanied by a decrease in degree of crystallinity (χ) and/or the glass transition temperature (T_g). Since decreases in χ and T_g are likely to improve mechanical properties like U_T, it difficult to understand the direct effects of H-bonds on the mechanical properties of glassy polymers using semicrystalline PVA. To overcome this doctoral student Adwait Gaikwad and Dr. Kolluru studied the mechanical behavior of amorphous, glassy state polyvinyl pyrrolidone (PVP), H-bonded

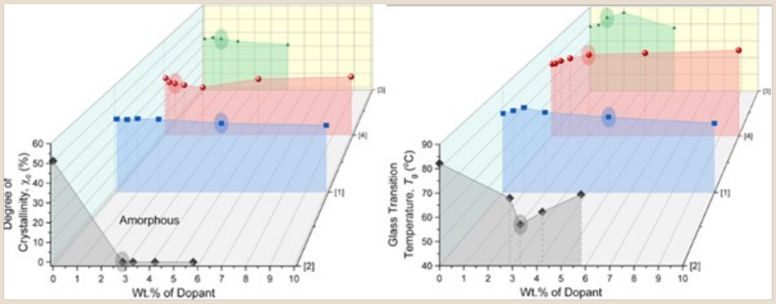

Figure 1. Changes in degree of crystallinity (χ) and glass transition temperature (T_g) of semicrystalline PVA with increasing small proton donor concentration from published literature ([1] X. Xu *et al.*, *Macromolecules* **54** (2021); [2] W. Niu et al., *ACS Appl. Mater. Interfaces* **12** (2020); [3] P. Song *et al.*, *Macromolecules.* **48** (2015); [4] P. Song *et al.*, *ACS Macro Lett.* **2** (2013)). Filled ovals identify the proton donor concentration at which optimal σ_f and U_T were observed in each study.

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Continues from page 1—Simultaneously Tougher and Thermally More Stable Hydrogen Bonded Polymer Glasses. Dr. Pavan Kolluru, MSEN

through tannic acid (TA). By way of uniaxial tension experiments on large sub-micron scale fibers (i.e., with diameters greater than 500 nm) electrospun PVP-TA with varying TA concentrations, they showed that H-bonding can directly and simultaneously improve the strength and toughness of the polymer, which is deep in the glassy state. This material system also enabled a systematic study of the impact of H-bonding on the elastic and plastic deformation, revealing differences in their trends with H-bonding (published here: https://doi.org/10.1002/mame.202300313). Elastic properties (such as elastic modulus, yield strength and resilience), depicted a monotonic increase with increasing TA content (i.e. increasing H-bond density). On the other hand, plastic properties (hardening modulus, failure strength, toughness and ductility) improved initially before reaching an optimal value, beyond which further addition of TA degraded the behavior, until the fibers eventually transition from ductile-to-brittle deformation (i.e. no plastic deformation). This indicated differences in the molecular mechanisms through which H-bonding is affected these two different deformation regimes. The non-monotonic changes in plastic deformation response were attributed to the beneficial effects of H-bond induced crosslinking while the detrimental effects of entanglement loss arising due to the addition of a small, non-entangling TA molecule. More importantly, as depicted in Figure 2, new materials design charts of T_g vs. mechanical properties from this study showed that amorphous H-bonded PVP-TA produce simultaneous improvement in toughness and thermal stability (T_g). From a technological standpoint, such a simultaneous increase in thermal stability and mechanical behavior helps develop new lightweight materials which can operate at higher temperatures, with reduced physical aging (and associated mechanical property degradation). As shown in these charts, traditional engineering plastics and even the previously studied semicrystalline and glassy H-bonded glassy PVA, do not exhibit such a simultaneous improvement in toughness/ductility and T_g.

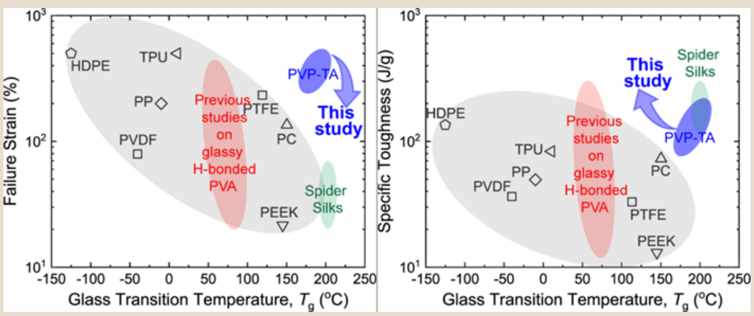
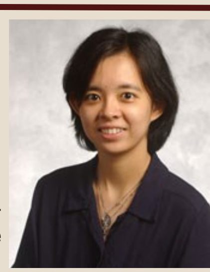


Figure 2. New material design charts showing ductility (left) and toughness (right) as a function of the glass transition temperature for general engineering plastics, H-bonded glassy PVA, spider silks and the amorphous glassy PVP-TA from the current study.

Kerfed wood composites: Interplay between geometry, material, aesthetic, and functionality

Anastacia Muliana
Mechanical Engineering



Modern architecture faces the growing demands of sustainable and high-performance building construction while ensuring aesthetic design freedom. Wood is a versatile and renewable material with a lower carbon footprint when compared to concrete and steel, making it a great choice for sustainable building construction. Its aesthetic quality also makes wood a natural choice for freeform structures. This drives the development of engineered wood materials, such as glued laminated (glulam), plywood, medium-density fiber (MDF), high-density fiber (HDF), cross-laminated timber (CLT), etc. Traditional building materials such as steel, aluminum, concrete, wood, and glass are not flexible enough to construct freeform shapes easily. The current manufacturing methods require making molds, casting individual modules, and joining them together, which is time-consuming, expensive, and produces a lot of waste. We are searching for a different fabrication method that involves using panels that can be shaped into various complex geometries. This flexibility is achieved by cutting solid panels with controlled microstructural patterns, which is known as kerfing. **Figure 1** shows an example of a kerf composite wood made of MDF. Laser cutting a periodic hexagonal pattern of unit cells creates a flexible and moldable wood panel. By varying the cutting density of the panel, a non-uniform distribution of flexibility is obtained. This allows for complex geometries to be spontaneously formed. Importantly, the unit cells in the kerf panel are continuously connected. This minimizes the number of joints and material waste, and enables the generation of nearly seamless freeform shapes.

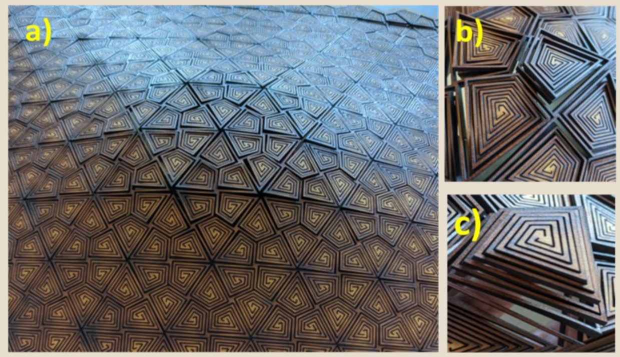


Figure 1 Kerf structures with macro-micro scale topology: a) kerf MDF panel, b) unit cell topology, and c) single cell reconfiguration

Working with wood composites is challenging due to their nonlinear and inelastic mechanical properties as well as their heterogeneous and anisotropic characteristics. In this study, we focus on using Medium-Density Fiberboard (MDF), which is made by combining chopped wood fibers with epoxy resin. The combination of epoxy resin and wood fibers creates a viscoelastic material, which can affect the shape and functional performance of kerf structures over time. To better understand this behavior, we conducted creep tests under uniaxial tension to explore the viscoelastic responses of MDF kerf unit cells. **Figure 2** (left) illustrates the MDF kerf unit cells with a side length of 1 inch and different cut densities. We refer to the cut density as a fractional order of repeating cuts in a cell. The lowest cut density (order 1) results in stiffer structures with higher load bearing. Increasing the order of cut density leads to more flexible surfaces at the expense of load-bearing capacity. We used an MDF panel with a thickness of 0.125 inches and laser cut the panel with a cut gap of 0.015 inches. Fillets of a radius of 0.004 in. are considered in all the unit cells at all the corners to avoid stress concentration that can cause failure. To describe the deformation of kerf unit cells, we use a nonlinear viscoelastic beam structural element with a rectangular cross-section. The nonlinear beam elements allow for axial stretching, transverse shearing, and large rotation bending and twisting. **Figure 2** (right) shows the creep responses of the kerf unit cells. The flexible unit cell (fractional cut order 3) experiences significant creep deformations. While engineering wood is known for their inherent viscoelatic material, adding kerf patterns can further enhance the overall material damping ability. We have created a kerf panel by controlling kerf topology, which involves determining the cut density orders and their arrangement based on the desired freeform shape. To demonstrate this process, we have taken a dome shape as an example, as shown in **Figure 3**. The desired freeform shapes can be achieved by defining a mapping function that maps a point in the undeformed state to the deformed state. From this mapping function, we can determine various measures of curvatures and corresponding deformation gradients. Using the deformation gradient, we can calculate the corresponding strain measures and stresses in the kerf panel, which are then used to decide on a suitable kerf topology. Currently, a manual trial-and-error process is being used

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continues from page 2 *"Kerfed wood composites: Interplay between geometry, material, aesthetic, and functionality"* Dr. Anastacia Muliana, MEEN

to determine the optimal topological arrangement. However, future optimization tools will enhance this process. The deformed shape and load-bearing response are also shown in **Figure 3**, highlighting the ability to create a high curvature shape in a narrow region via controlling kerf cut density.

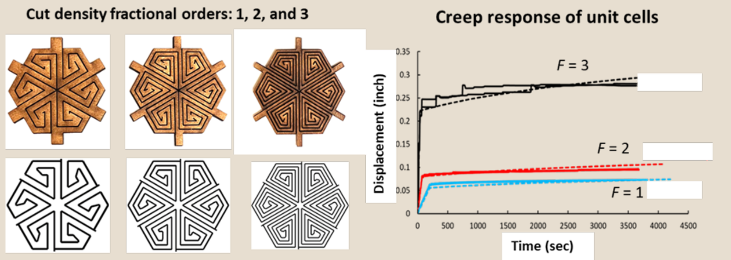

Figure 2 Left: unit cells with different orders of cut density out of MDF and their corresponding beam element models. Right: creep responses of the unit cells comparing responses from the model (solid lines) and experiments (dashed lines). Ref: Darnal et al. 2023.

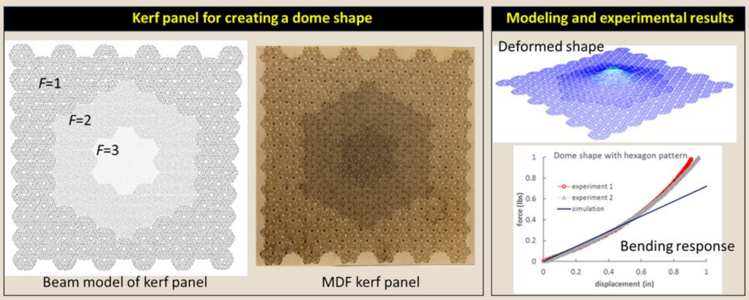

Figure 3 Left: a kerf panel with varying orders of cut densities to achieve a dome shape. Right: bending response generating a dome shape.

The kerf topology, with its architected nature, is capable of displaying a stress wave manipulation that is attributed to its cell periodicity and flexibility (refer to **Figure 1**). In fact, it can promote internal resonant mechanisms from dynamic excitations. Due to its microstructural complexity, the kerf topology enables the steering and trapping of waves at different frequencies, as seen from stress wave propagation responses in a kerf panel from dynamic excitation loadings (see **Figure 4**). This feature is useful in controlling wave propagation in the kerf panel and generating freeform shapes simultaneously. The kerf topology's ability to manipulate wave propagation is beneficial in civil infrastructures exposed to various dynamic events such as ground motions, winds, and acoustic loadings.

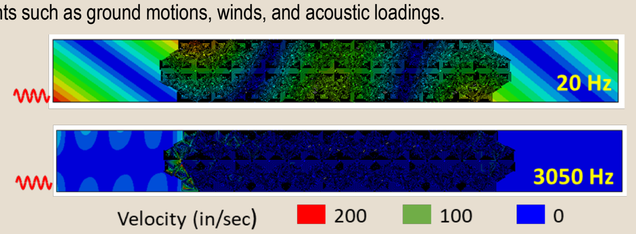

Figure 4 Stress wave propagation responses of kerf panel at different excitation frequencies.

We further explore the impact of kerf structures on soundscape characteristics. Our intention was to control sound environment of the lounge area of Autodesk Gallery in San Francisco that was not conducive to intimate and private conversations in the open-plan layout. The goal was to provide an aesthetically pleasing wall out of kerfing, to improve the acoustic performance of the lounge by creating a diffuse soundscape within the gallery's echoey space (Bohrani et al., 2022). The design was inspired by Muqarnas vaulted ceilings in Āli Qapu Palace's music hall (**Figure 5**). To control the sonic characteristics of the lounge area, we need to efficiently diffuse sound by facilitating sound focusing from different wall panels, i.e., reflecting and concentrating sound waves from and near the surface. Here, we explore the interplay between geometry, material, and functionality to achieve desired visual, aural, and structural integrity of the kerf panel. To support the out-of-plane topological transformation of flat kerf panels we design attractors at different heights, to control the curvature of the surface (**Figure 6**). In this way, the global load bearing capacity of the surface and its acoustic characteristics can be tuned, i.e., increasing curvature enhances surface tension, improves overall bending stiffness, and brings sound diffusion closer to the surface.

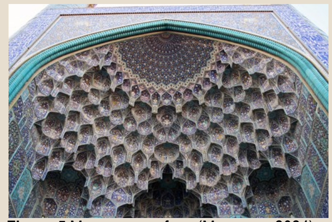

Figure 5 Muqarnas surface (Muqarnas 2024)

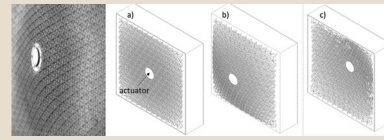

Figure 6 Attractors to change the curvature locally

The effectiveness of kerf structures in altering the reverberation time (RT60) has been demonstrated through a measurement before and after installation of the kerf panel, following the ISO 3382-2 standard measurement (Bohrani et al., 2022). The measurements were taken at six fixed receiver positions and frequencies ranging from 125 Hz to 4000 Hz. The average values of RT60 with and without the kerf surface are illustrated in **Figure 5**. The installation of kerf structures in the room significantly reduced the reverberation time, thus mitigating echoing in the lounge area.

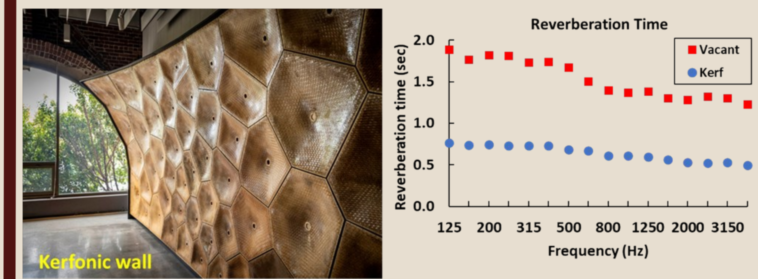

Figure 5 Left: a kerf panel of freeform geometry for controlled indoor acoustic. Right: the effect of kerf structure on RT60 in a room. Ref: Bohrani et al., 2022

We demonstrate the idea of using a kerfing approach to create an architectural structure out of engineered wood that blends aesthetic and functional performances, i.e., acoustic characteristics and structural integrity. This was achieved by applying the fundamental engineering knowledge of differential geometry, mechanics of viscoelastic materials, structural analysis, acoustic wave propagation, and fabrication constraints via laser cutting.

Acknowledgment: This work is in collaboration with Dr. Negar Kalantar from California College of the Arts. The graduate students involved in this project are Dr. Zaryab Shahid and Aryabhat Darnal. We thank Dr. Ed Green from B&K for helping with testing room acoustic performance. Part of this project is sponsored by the US National Science Foundation. We also thank the TAMU High-Performance Research Computing for the computational support.

References:

Bohrani A, Kalantar N, Rezaei E, Muliana A, Shahid Z, and Green E (2022), "The Sound of Kerfing: A New Approach to Integrating Geometry, Materials, and Acoustics to Build Invisibles," Proceedings ACADIA 2022 Hybrids and Haecceities, University of Pennsylvania | Philadelphia, PA, October 26-29

Darnal A, Shahid A, Kalantar N, and Muliana A (2023), "The Influence of Inelastic Materials on Freeform Kerf Structures" Thin-Walled Structures, 193, 111292

Muqarnas. (2024, April 9). In *Wikipedia*. https://en.wikipedia.org/wiki/Muqarnas

SPE Spring 2024 scholarship recipients recognized at the PTIC meeting on April 19th, 2024, as follows:

L-R: Nicholas Starvaggi, MSEN received the SPE Henry Kahn memorial scholarship; Dr. Dave Hansen, SPE Liaison; and Sarah Hilburgh, MSEN received the SPE Dale Walker memorial scholarship.

L-R: Xiuzhu Zhu, MSEN received a SPE scholarship; Donna Davis, SPE Liaison; and Smita Shivraj Dasari, CHEN received a SPE scholarship

CONGRATULATIONS to all these students!

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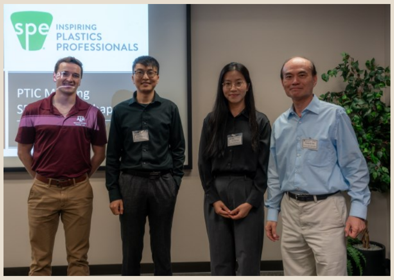
PTC welcomes the newest member to the Polymer Technology Industrial Consortia—PTIC. Please welcome: EVANTIC

EVANTIC

The PTIC student poster session was held on April 18th-19th, 2024 with the following students placing in the event. PTC would like to Congratulate these students for enthusiastically showcasing their research to the Polymer Industry.



PLACE-MENT	Students name	Major	PTIC poster title
1st	Nicholas Starvaggi	MSEN	"Microcapsule Fabrication by ATRP at the Interface of Non-Aqueous Emulsions"
2nd	Huaixuan Cao	CHEN	"Structured MXene/polymer composites from Pickering emulsion templating"
3rd	Yinying Hua	CHEN	"Improving Propylene/Propane Separation Performances of Asymmetric Mixed-Matrix Membranes through Additive-Assisted In-Situ ZIF-8 Formation"

WHOOP! GIG 'EM AGGIES WHOOP!

SPE STUDENT CHAPTER officers for 2023-24

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Polymer Specialty Certificate Updates

Students that have applied for the Polymer Specialty Certificate	87
Students that have received the Polymer Specialty Certificate	75

For more information, please visit: http://ptc.tamu.edu/polymer-specialty-certificate/

Have Questions?

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PTC Polymer Technology Consortia
Materials Science & Engineering

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